

Moving boundary problem for the detachment in multispecies biofilms

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Abstract The work presents the qualitative analysis of the free boundary value problem related to the detachment process in multispecies biofilms. In the framework of continuum approach to one-dimensional mathematical modelling of multispecies biofilm growth, we consider the system of nonlinear hyperbolic partial differential equations governing the microbial species growth, the differential equation for the biomass velocity, the differential equation that governs the free boundary evolution and also accounts for detachment, and the elliptic system for substrate dynamics. The characteristics are used to convert the original moving boundary equation into a suitable differential equation useful to solve the mathematical problem. We also provide another form of the same equation that could be used in numerical applications. Several properties of the solutions to the free boundary problem are shown, such as positiveness of the functions that describe the microbial concentrations and estimates on the characteristic functions. Uniqueness and existence of solutions are proved by introducing a suitable system of Volterra integral equations and using the fixed point theorem.

Keywords Free boundary value problems · Nonlinear hyperbolic partial differential equations · Detachment model · Multispecies biofilm continuum model

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1 Introduction

The first biofilm was discovered in 1600s by the Dutch scientist Anton Van Leeuwenhoek, when he observed with his microscope a microbial community in the plaque scraped from his teeth. The modern definition of bacterial biofilm was given recently by Costerton in 1999 and states: *structured community of bacterial cells enclosed in a self-produced polymeric matrix and adherent to an inert or living surface* [1].

Biofilms are found in extremely varied environments, both natural and artificial, and in diverse hydrodynamic conditions. They are usually characterized by the presence of multiple species, which experience different living conditions due to the establishment of substrate gradients and specific micro-environments. Biofilms are widely used in industrial and engineering applications: biofuels and electricity production, bioremediation, water purification and wastewater treatment. However, they have also negative occurrences as they can be considered a leading cause of chronic infections, biocorrosion and biofouling.

Literature on mathematical modelling of biofilms presents continuum or discrete approach [2–6]. For engineering practice, 1D continuum models have been widely used to describe biofilm dynamics, in particular for engineering design of biofilm reactors for wastewater treatment plants, see [7] for a review.

We consider multispecies biofilm growth in the framework of 1D continuum approach. Mathematical modelling leads to discuss free boundary value problems, where the biofilm thickness $L(t)$ is the moving boundary. The evolution of the free boundary of course depends on biomass velocity u by which the biomass is displaced respect to the growth direction. In addition, it depends on detachment and attachment biomass flux from bulk liquid, denoted by σ_d and σ_a , respectively. The function σ_d depends on L^2 *de facto* as outlined in [8]. Therefore, the detachment is relevant for mature biofilms and negligible in the first phase of biofilm formation. The detachment represents the primary process that limits biofilm accumulation. The detachment problem was first discussed in [8], where the analysis was mainly carried out on single-species biofilm and then partially applied to multispecies biofilms.

In this work we discuss the detachment free boundary value problem for multispecies biofilms constituted by any number of microbial species. The main results are properties of solutions and existence and uniqueness theorem. We consider a methodology based on the characteristics that was successfully used in previous works for the free boundary problem related to the initial phase of biofilm formation when the detachment is negligible, [9], and then generalized to the free boundary problem where $\sigma_d = \sigma_a = 0$, [10].

We first focus our analysis on the essential mathematical problem and consider the system of nonlinear hyperbolic partial differential equations that governs multispecies biofilm growth and neglect the semi-linear parabolic partial differential equations that govern the substrate evolution within the biofilm. This assumption allows us to not further complicate the system with equations that do not alter the hyperbolic feature

of the free boundary problem. We then use the previous results to discuss the general situation of nonlinear coupled hyperbolic parabolic free boundary problem. We show the positiveness of the functions related to the microbial species and provide estimates on the characteristic functions that are useful to go back from the characteristic coordinates to the physical ones. Moreover, it is proved that the sum of volume fractions is saved on time. This result is also important in numerical simulations since it could be used to check the error at each time step.

Let us add that, as for most 1D biofilm models, the above mentioned problem has been extensively studied in special situations through numerical simulations, e.g. [11–13]. Therefore, the qualitative analysis discussed in this work, apart from its intrinsic interest, also provides a solid base to numerical findings.

In Sect. 2 the free boundary problem is presented, the variables defined, the main assumptions are discussed, the initial and boundary conditions are introduced. In Sect. 3 the equation for the moving boundary is derived. The characteristics are used to convert the original moving boundary equation into a suitable differential equation useful to prove the existence and uniqueness theorem. We also provide another form of the same equation that could be used in numerical applications. In addition, it is shown that the present problem can include the one discussed in [10] as special case. Section 4 is devoted to properties of the solutions to the free boundary value problem. The main theorem is proved in Sect. 5. The number n of species into the biofilm is assumed to be arbitrary. The hypotheses on the initial data are quite general and in agreement with the biology. The original differential equations are converted to Volterra integral equations. Uniqueness and existence of solutions are achieved by the fixed point theorem in the class of continuous functions. Section 6 is devoted to the general complete problem. By using the results of Sect. 5, the equations for substrate dynamics are converted to integral equations and discussed. Conclusion is the last brief section.

2 Mathematical model for the detachment process

Let us refer to 1D continuum approach for multispecies biofilm formation and growth, [2,3,7]. Denote by z the one-dimensional biofilm growth direction and assume that biofilm support, substratum, is placed at $z = 0$. Consider a biofilm constituted by n species and let $X_i(z, t)$ be the concentration of microorganisms i . The biofilm growth is governed by the following system of nonlinear partial differential equations for the microbial concentrations

$$\frac{\partial X_i}{\partial t} + \frac{\partial}{\partial z}(uX_i) = \rho_i r_{M,i}, \quad i = 1, \dots, n, \quad 0 \leq z \leq L(t), \quad t > 0, \quad (2.1)$$

where $u(z, t)$ is the biomass velocity, ρ_i the constant density of the microbial species i , and $L(t)$ the biofilm thickness which is the free boundary of the mathematical problem. The function $u(z, t)$ satisfies the following equation

$$\frac{\partial u}{\partial z} = \sum_{i=1}^n r_{M,i}, \quad 0 < z \leq L(t), \quad t \geq 0. \quad (2.2)$$

The function $L(t)$ satisfies the following equation

$$\dot{L}(t) = u(L(t), t) - \sigma_d(L(t)), \quad t > 0, \quad (2.3)$$

where $\sigma_d(L(t))$ is the detachment biomass flux from biofilm to bulk liquid. The most used expression for σ_d is the following, [8],

$$\sigma_d(L) = \sigma_0 L^2, \quad \sigma_0 = \text{constant}. \quad (2.4)$$

Therefore, the detachment biological process is relevant for mature biofilms, when L is large.

The term $r_{M,i}$ in Eq. (2.1) represents the specific growth rate of species i . The following expression is generally assumed for $r_{M,i}$, [2,3,7],

$$r_{M,i} = \sum_{j=1}^n \mu_{ij} X_j, \quad (2.5)$$

where the specific growth rate functions μ_{ij} depend on the substrates S_h , $h = 1, \dots, m$, diffusing into the biofilm. The dependence on S_h is more frequently nonlinear, although linear dependence is admissible, according to special kinetics. However, nonlinear dependence is assumed in this work. Also, more complex expressions for $r_{M,i}$ are present in literature, for example, when the biological process of the invasion of new species into an already constituted biofilm is modelled, [14,15].

In all these cases further equations should be introduced. For example, in the case (2.5) the equations governing substrate dynamics should be introduced. However, by considering Eq. (2.3) it is apparent that the free boundary depends on biomass velocity u that in turns depends on the nonlinear hyperbolic system (2.1). All the other equations are important when specific biological situations are considered and studied but they do not change the hyperbolic feature of the free boundary problem. Therefore, we first focus our analysis on the essential mathematical problem and assume

$$r_{M,i} = r_{M,i}(z, t, \mathbf{X}), \quad \mathbf{X} = (X_1, \dots, X_n), \quad i = 1, \dots, n. \quad (2.6)$$

Then, the general situation where $r_{M,i}$ also depends on substrates

$$r_{M,i} = r_{M,i}(z, t, \mathbf{X}, \mathbf{S}), \quad \mathbf{S} = (S_1, \dots, S_m), \quad i = 1, \dots, n, \quad (2.7)$$

will be easily discussed in Sect. 6.

Now, the initial and boundary conditions for system (2.1)–(2.3) are presented. They are quite general and state

$$X_i(z, 0) = \varphi_i(z) \geq 0, \quad 0 \leq z \leq L(0), \quad i = 1, \dots, n, \quad (2.8)$$

$$L(0) = L_0 > 0, \quad (2.9)$$

$$u(0, t) = 0, \quad t > 0. \quad (2.10)$$

The completely arbitrary functions φ_i in (2.8) describe the initial status of the biofilm. According to the biological problem they must be assigned nonnegative. The positive constant L_0 in (2.9) denotes the initial biofilm thickness. The condition in (2.10) indicates that there is no biomass flux at the support.

Finally, Eqs. (2.1)–(2.3) are briefly commented and references are provided for detail [2, 10]. System (2.1) derives from local mass balance. It was first presented in [2]. System (2.1) is generally used to describe the dynamics of not only the active microbial species but of all the particulate components, including inert biomass and extracellular polymeric substances (EPS), which constitute the biofilm. An equivalent alternative system can be used if the volume fraction $f_i(z, t)$ of microbial species i is considered. Indeed, it is

$$X_i(z, t) = \rho_i f_i(z, t), \quad i = 1, \dots, n, \quad 0 \leq z \leq L(t), \quad t > 0, \quad (2.11)$$

and system (2.1) can be rewritten as

$$\frac{\partial f_i}{\partial t} + \frac{\partial}{\partial z}(u f_i) = r_{M,i}, \quad i = 1, \dots, n, \quad 0 \leq z \leq L(t), \quad t > 0. \quad (2.12)$$

Equation (2.2) is obtained from (2.12) by summing on i and using $\sum_{i=1}^n f_i = 1$. It regulates the expansion velocity of the microbial mass. Equation (2.3) describes the free boundary evolution. It derives from global mass balance by taking into account the detachment flux, [10].

3 Moving boundary

In this section a suitable equation for the moving boundary is deduced. Consider system (2.1) and the characteristic-like lines $z = c(z_0, t)$ defined by

$$\frac{\partial c}{\partial t}(z_0, t) = u(c(z_0, t), t), \quad c(z_0, 0) = z_0, \quad z_0 \in [0, L_0], \quad t > 0. \quad (3.1)$$

From the definition above it follows that the characteristic for $z_0 = 0$ is

$$z = c(0, t) = 0. \quad (3.2)$$

Indeed, from definition (3.1)

$$\frac{\partial c}{\partial t}(0, t) = u(c(0, t), t), \quad c(0, 0) = 0.$$

Since $u(0, t) = 0$, as stated in (2.10), it follows (3.2).

Consider Eq. (2.2)

$$\frac{\partial u}{\partial z}(z, t) = g(z, t, \mathbf{X}(z, t)), \quad 0 < z \leq L(t), \quad t \geq 0, \quad (3.3)$$

where the following definition has been used for brevity

$$g(z, t, \mathbf{X}) = \sum_{i=1}^n r_{M,i}. \quad (3.4)$$

From (3.3) it follows

$$\frac{\partial u(c(z_0, t), t)}{\partial z_0} = g(c(z_0, t), t, \mathbf{x}(z_0, t)) \frac{\partial c}{\partial z_0}(z_0, t), \quad (3.5)$$

where

$$\mathbf{x}(z_0, t) = \mathbf{X}(c(z_0, t), t). \quad (3.6)$$

Integrating (3.5) yields

$$u(c(z_0, t), t) = \int_0^{z_0} g(c(\zeta_0, t), t, \mathbf{x}(\zeta_0, t)) \frac{\partial c}{\partial \zeta_0}(\zeta_0, t) d\zeta_0, \quad (3.7)$$

where Eqs. (2.10) and (3.2) have been used. Substitute (3.7) in Eq. (3.1)₁ and integrate with respect to time with initial condition (3.1)₂

$$c(z_0, t) = z_0 + \int_0^t d\tau \int_0^{z_0} g(c(\zeta_0, \tau), \tau, \mathbf{x}(\zeta_0, \tau)) \frac{\partial c}{\partial \zeta_0}(\zeta_0, \tau) d\zeta_0. \quad (3.8)$$

Hence,

$$\frac{\partial c(z_0, t)}{\partial z_0} = 1 + \int_0^t g(c(z_0, \tau), \tau, \mathbf{x}(z_0, \tau)) \frac{\partial c}{\partial z_0}(z_0, \tau) d\tau. \quad (3.9)$$

If we introduce the following position

$$U(z_0, t) = u(c(z_0, t), t), \quad (3.10)$$

then Eqs. (3.7)–(3.9) can be written as

$$U(z_0, t) = \int_0^{z_0} g(c(\zeta_0, t), t, \mathbf{x}(\zeta_0, t)) \frac{\partial c}{\partial \zeta_0}(\zeta_0, t) d\zeta_0, \quad (3.11)$$

$$c(z_0, t) = z_0 + \int_0^t U(z_0, \tau) d\tau, \quad (3.12)$$

$$\frac{\partial c(z_0, t)}{\partial z_0} = 1 + \int_0^t \frac{\partial U(z_0, \tau)}{\partial z_0} d\tau, \quad (3.13)$$

respectively.

Denote by

$$w = w(t), \quad (3.14)$$

the initial point of the characteristic that assumes the value $L(t)$ at the time t ,

$$L(t) = c(w(t), t). \quad (3.15)$$

Using (3.15) in moving boundary Eq. (2.3) yields

$$\begin{aligned} \dot{c}(w(t), t) &= \dot{L}(t) = u(c(w(t), t), t) - \sigma_d(c(w(t), t)) \\ &= U(w(t), t) - \sigma_d(c(w(t), t)). \end{aligned} \quad (3.16)$$

Note that the function w plays the same role as z_0 for the characteristic passing through L at time t and it is $w(0) = L_0$. Therefore, if we apply the general definition (3.12) for $z_0 = w(t)$, we get

$$c(w(t), t) = w(t) + \int_0^t U(w(t), \tau) d\tau. \quad (3.17)$$

Hence, after differentiating with respect to t ,

$$\dot{c}(w(t), t) = \dot{w}(t) + U(w(t), t) + \int_0^t \dot{w}(t) \frac{\partial U(w(t), \tau)}{\partial z_0} d\tau. \quad (3.18)$$

From (3.16) and (3.18) we get

$$\dot{w}(t) + U(w(t), t) + \int_0^t \dot{w}(t) \frac{\partial U(w(t), \tau)}{\partial z_0} d\tau = U(w(t), t) - \sigma_d(c(w(t), t)). \quad (3.19)$$

Hence, the desired differential equation for $w(t)$

$$\dot{w}(t) \frac{\partial c}{\partial z_0}(w(t), t) = -\sigma_d(c(w(t), t)), \quad t > 0. \quad (3.20)$$

An integral equation for $w(t)$ is easily obtained by integrating with respect to time with initial condition $w(0) = L_0$

$$w(t) = L_0 - \int_0^t \sigma_d(c(w(\tau), \tau)) d\tau + \int_0^t U(w(\tau), \tau) d\tau - \int_0^t U(w(t), \tau) d\tau, \quad t > 0. \quad (3.21)$$

Some comments are necessary on Eqs. (3.20) and (3.21). After determining the characteristics, besides the other functions involved, they allow us to find the free boundary. Equation (3.20) can be solved with respect $\dot{w}(t)$ since $\partial c / \partial z_0 \geq 1$, as proved in Sect. 4. Equation (3.20) is very useful in the numerical approach to the problem. Equation (3.21) will be used in the existence and uniqueness theorem proved in Sect. 5.

We conclude the present section with a remark on the special solution of Eq. (3.21) connected with the problem discussed in [9] where the detachment was neglected and

$$\sigma_d = 0. \quad (3.22)$$

Remark 3.1 Under assumption (3.22) the Eq. (2.3) for the free boundary writes

$$\dot{L}(t) = u(L(t), t), \quad L(0) = L_0. \quad (3.23)$$

By comparing the last equation with Eq. (3.1) that defines the characteristic lines, we immediately realize that the free boundary is the same as the characteristic line starting from L_0 . In other words, for the special case (3.22) the function $w(t)$ is identically equal to L_0

$$w(t) = L_0. \quad (3.24)$$

Therefore, Eq. (3.21) should admit the solution (3.24) under assumption (3.22). This is true. Indeed, in such a case Eq. (3.21) writes

$$w(t) = L_0 + \int_0^t U(w(\tau), \tau) d\tau - \int_0^t U(w(t), \tau) d\tau,$$

with solution given by (3.24). Uniqueness and existence theorem for Eq. (3.21) will be proved in Sect. 5.

4 Properties of solutions to the free boundary problem

In this section we anticipate some properties of solutions to the free boundary value problem stated in Sect. 2. A uniqueness and existence theorem will be provided in the next section. The hypotheses of theorem are assumed to be fulfilled in proving the properties so that the solution to the free boundary problem exists.

Consider system (2.1) rewritten by using definition (3.4)

$$\frac{\partial X_i}{\partial t} + u \frac{\partial X_i}{\partial z} = \rho_i r_{M,i} - X_i g, \quad i = 1, \dots, n, \quad 0 \leq z \leq L(t), \quad t > 0. \quad (4.1)$$

Consider the characteristics (3.1) and obtain

$$\dot{x}_i(z_0, t) = F_i(c(z_0, t), t, \mathbf{x}(z_0, t)), \quad i = 1, \dots, n, \quad z_0 \in [0, L_0], \quad t > 0, \quad (4.2)$$

where $\mathbf{x}(z_0, t)$ was introduced in (3.6) and

$$F_i(c(z_0, t), t, \mathbf{x}(z_0, t)) = \rho_i r_{M,i} - x_i g. \quad (4.3)$$

The initial condition for $\mathbf{x}(z_0, t)$ is easily derived from (2.8)

$$x_i(z_0, 0) = X_i(c(z_0, 0), 0) = X_i(z_0, 0) = \varphi_i(z_0), \quad i = 1, \dots, n, \quad z_0 \in [0, L_0]. \quad (4.4)$$

Integrating (4.2) leads to the following system of integral equations

$$x_i(z_0, t) = \varphi_i(z_0) + \int_0^t F_i(c(z_0, \tau), \tau, \mathbf{x}(z_0, \tau)) d\tau, \quad i = 1, \dots, n, \quad z_0 \in [0, L_0], \quad (4.5)$$

which incorporate the initial conditions (4.4). The integral version for Eq. (2.2) was already provided in (3.11). It is rewritten for convenience

$$U(z_0, t) = \int_0^{z_0} g(c(\zeta_0, t), t, \mathbf{x}(\zeta_0, t)) \frac{\partial c}{\partial \zeta_0}(\zeta_0, t) d\zeta_0, \quad z_0 \in [0, L_0], \quad t > 0, \quad (4.6)$$

noting that the boundary condition (2.10) is included. Also the following three equations are rewritten for convenience

$$c(z_0, t) = z_0 + \int_0^t d\tau \int_0^{z_0} g(c(\zeta_0, \tau), \tau, \mathbf{x}(\zeta_0, \tau)) \frac{\partial c}{\partial \zeta_0}(\zeta_0, \tau) d\zeta_0, \quad z_0 \in [0, L_0], \quad t > 0, \quad (4.7)$$

$$\frac{\partial c(z_0, t)}{\partial z_0} = 1 + \int_0^t g(c(z_0, \tau), \tau, \mathbf{x}(z_0, \tau)) \frac{\partial c}{\partial z_0}(z_0, \tau) d\tau, \quad z_0 \in [0, L_0], \quad t > 0, \quad (4.8)$$

$$w(t) = L_0 - \int_0^t \sigma_d(c(w(\tau), \tau)) d\tau + \int_0^t U(w(\tau), \tau) d\tau - \int_0^t U(w(t), \tau) d\tau, \quad t > 0. \quad (4.9)$$

System (4.5)–(4.9) has a unique solution in the functional class of continuous functions defined on

$$\Omega\{(z_0, t) : z_0 \in [0, L_0], \quad t \in [0, T], \quad L_0, T > 0\}, \quad (4.10)$$

as proved in Sect. 5, Theorem 1. This result is assumed in the following where several properties of solutions to system (4.5)–(4.9) are provided. Some properties require the function g in (3.4) must be positive

$$g(z, t, \mathbf{X}) \geq 0. \quad (4.11)$$

We outline that assumption (4.11) is satisfied in most biological processes related to biofilm growth, e.g. [2, 7].

Property 1 Suppose that hypotheses of Theorem 1 are satisfied. Then, under assumption (4.11) it results

$$\frac{\partial c(z_0, t)}{\partial z_0} \geq 1, \quad z_0 \in [0, L_0], \quad t \in]0, T]. \quad (4.12)$$

Proof Inequality (4.12) follows from integral equation (4.8).

Property 2 Under the same hypotheses as Property 1 it results

$$U(z_0, t) \geq 0, \quad z_0 \in [0, L_0], \quad t \in]0, T]. \quad (4.13)$$

Proof Estimate (4.13) follows from integral Eq. (4.6) and Property 1.

Property 3 Under the same hypotheses as Property 1 it results

$$c(z_0, t) \geq 0, \quad z_0 \in [0, L_0], \quad t \in]0, T]. \quad (4.14)$$

Proof Estimate (4.14) follows from integral Eq. (4.7) and Property 1.

Property 4 Under the same hypotheses as Theorem 1 it results

$$\sum_{i=1}^n f_i(z_0, 0) = 1 \Rightarrow \sum_{i=1}^n f_i(z_0, t) = 1. \quad (4.15)$$

Proof Let us rewrite integral Eq. (4.5) in terms of volume fractions defined in (2.11)

$$f_i(z_0, t) = \varphi_i(z_0)/\rho_i + \int_0^t (r_{M,i} - f_i g) d\tau, \quad i = 1, \dots, n. \quad (4.16)$$

Using the position

$$f(z_0, t) = \sum_{i=1}^n f_i(z_0, t)$$

and summing on i yields

$$f(z_0, t) = 1 + \int_0^t g(1 - f) d\tau, \quad (4.17)$$

since

$$\sum_{i=1}^n \varphi_i(z_0)/\rho_i = \sum_{i=1}^n f_i(z_0, 0) = 1. \quad (4.18)$$

Equation (4.17) admits the solution $f(z_0, t) = 1$ proving (4.15).

Property 5 Assume that hypotheses of Theorem 1 are satisfied and

$$\begin{aligned} F_i(c(z_0, t), t, \mathbf{x}(z_0, t)) &\geq 0, \quad z_0 \in [0, L_0], \quad t \in]0, T], \quad i = 1, \dots, n_1, \\ \varphi(z_0) + T \max_{(z_0, t)} |F_i| &\geq 0, \quad z_0 \in [0, L_0], \quad t \in]0, T], \quad i = n_1 + 1, \dots, n. \end{aligned} \quad (4.19)$$

$$(4.20)$$

Then

$$x_i(z_0, t) \geq 0, \quad i = 1, \dots, n. \quad (4.21)$$

Proof Estimate (4.21) follows from integral Eq. (4.5) under the natural hypothesis of positive initial microbial concentrations as stated in (2.8). Note that n_1 denotes the number of microbial species with increasing concentrations.

Remark 4.1 From the mathematical point of view, the most important result is (4.12), see Remark 5.1 at the end of Sect. 5. From the biological point of view, the main results are (4.13), (4.15) and (4.21). In addition, the result (4.15) could be used to estimate the error in numerical simulations.

5 Proof of uniqueness and existence theorem

In order to obtain more compact equations, let us introduce the following definitions

$$x_{n+1} = c, \quad x_{n+2} = \partial c / \partial z_0, \quad x_{n+3} = U, \quad x_{n+4} = w,$$

and redefine the vector \mathbf{x} as follows

$$\mathbf{x} = (x_1, \dots, x_n, x_{n+1}, \dots, x_{n+4}). \quad (5.1)$$

Therefore, Eq. (4.5) writes

$$x_i(z_0, t) = \varphi_i(z_0) + \int_0^t F_i(\tau, \mathbf{x}(z_0, \tau)) d\tau, \quad i = 1, \dots, n, \quad z_0 \in [0, L_0], \quad t > 0. \quad (5.2)$$

Equation (4.7) writes

$$x_{n+1}(z_0, t) = z_0 + \int_0^t d\tau \int_0^{z_0} F_{n+1}(\tau, \mathbf{x}(\zeta_0, \tau)) d\zeta_0, \quad z_0 \in [0, L_0], \quad t > 0, \quad (5.3)$$

where

$$F_{n+1} = g(c(\zeta_0, \tau), \tau, \mathbf{x}(\zeta_0, \tau)) \frac{\partial c}{\partial \zeta_0}(\zeta_0, \tau).$$

Equation (4.8) writes

$$x_{n+2}(z_0, t) = 1 + \int_0^t F_{n+2}(\tau, \mathbf{x}(z_0, \tau)) d\tau, \quad z_0 \in [0, L_0], \quad t > 0, \quad (5.4)$$

where

$$F_{n+2} = g(c(z_0, \tau), \tau, \mathbf{x}(z_0, \tau)) \frac{\partial c}{\partial z_0}(z_0, \tau).$$

Equation (4.6) writes

$$x_{n+3}(z_0, t) = \int_0^{z_0} F_{n+3}(t, \mathbf{x}(\zeta_0, t)) d\zeta_0, \quad z_0 \in [0, L_0], \quad t > 0, \quad (5.5)$$

where

$$F_{n+3} = g(c(\zeta_0, t), t, \mathbf{x}(\zeta_0, t)) \frac{\partial c}{\partial \zeta_0}(\zeta_0, t).$$

Equation (4.9) writes

$$\begin{aligned} x_{n+4}(t) = & L_0 - \int_0^t F_{n+4,1}(\tau, x_{n+4}(\tau)) d\tau \\ & + \int_0^t F_{n+4,2}(\tau, x_{n+4}(\tau)) d\tau - \int_0^t F_{n+4,3}(\tau, x_{n+4}(t)) d\tau, \quad t > 0, \end{aligned} \quad (5.6)$$

where

$$F_{n+4,1}(\tau, x_{n+4}(\tau)) = \sigma_d(c(w(\tau), \tau)), \quad (5.7)$$

$$F_{n+4,2}(\tau, x_{n+4}(\tau)) = U(w(\tau), \tau), \quad F_{n+4,3}(\tau, x_{n+4}(t)) = U(w(t), \tau). \quad (5.8)$$

Now, we can show the following theorem.

Theorem 1 Suppose that:

- (i) $x_k(z_0, t) \in C^0([0, L_0] \times [0, T_1])$, $L_0 > 0$, $T_1 > 0$, $k = 1, \dots, n+4$;
- (ii) $\varphi_i(z_0) \in C^0([0, L_0])$, $i = 1, \dots, n$;
- (iii) $|x_i - \varphi_i| \leq h_i$, $i = 1, \dots, n$; $|x_{n+1} - z_0| \leq h_{n+1}$; $|x_{n+2} - 1| \leq h_{n+2}$; $|x_{n+3}| \leq h_{n+3}$; $|x_{n+4} - L_0| \leq h_{n+4}$, where $h_k = \text{constant} > 0$, $k = 1, \dots, n+4$;
- (iv) $F_1, \dots, F_{n+3}, F_{n+4,1}, F_{n+4,2}, F_{n+4,3}$ are bounded and Lipschitz continuous with respect to x_k , $k = 1, \dots, n+4$,

$$M_j = \max |F_j|, \quad j = 1, \dots, n+3,$$

$$M_{n+4,i} = \max |F_{n+4,i}|, \quad i = 1, 2, 3, \quad M_{n+4} = \sum_{i=1}^3 M_{n+4,i},$$

$$|F_j(\tau, t, \mathbf{x}) - F_j(\tau, t, \tilde{\mathbf{x}})| \leq \lambda_j \sum_{k=1}^{n+4} |x_k - \tilde{x}_k|, \quad j = 1, \dots, n+3,$$

$$|F_{n+4,i}(\tau, t, \mathbf{x}) - F_{n+4,i}(\tau, t, \tilde{\mathbf{x}})| \leq \lambda_{n+4,i} \sum_{k=1}^{n+4} |x_k - \tilde{x}_k|, \quad i = 1, 2, 3,$$

when $(z_0, t) \in [0, L_0] \times [0, T_1]$ and the functions x_k satisfy the assumptions (i)–(iii).

Then, integral system (5.2)–(5.6) has a unique solution $x_k \in C^0([0, L_0] \times [0, T])$, $k = 1, \dots, n+4$, where

$$T = \min \left\{ T_1, \frac{h_1}{M_1}, \dots, \frac{h_n}{M_n}, \frac{h_{n+1}}{L_0 M_{n+1}}, \frac{h_{n+2}}{M_{n+2}}, \frac{h_{n+4}}{M_{n+4}} \right\}, \quad M_{n+3} L_0 \leq h_{n+3}.$$

Proof Denote by Ω the space of continuous functions $x_i(z_0, t)$, $z_0 \in [0, L_0]$, $t \in [0, T]$. Introduce the norm

$$||\mathbf{x}|| = \sum_{k=1}^{n+4} \max_{\Omega} \exp(-\gamma_1 t - \gamma_2 z_0) |x_k|,$$

where γ_1, γ_2 are positive constants that will be fixed later on.

Consider the map $\mathbf{y} = \mathbf{A}\mathbf{x}$, $y_k =$ right hand side of Eqs. (5.2)–(5.6). Let us prove that \mathbf{A} maps Ω into itself. Indeed,

$$\begin{aligned} |y_i - \varphi_i| &\leq M_i T \leq h_i, \quad i = 1, \dots, n, \\ |y_{n+1} - z_0| &\leq M_{n+1} T L_0 \leq h_{n+1}, \\ |y_{n+2} - 1| &\leq M_{n+2} T \leq h_{n+2}, \\ |y_{n+3}| &\leq M_{n+3} L_0 \leq h_{n+3}, \\ |y_{n+4} - L_0| &\leq M_{n+4} T \leq h_{n+4}. \end{aligned}$$

Consider $\tilde{\mathbf{x}} \in \Omega$ and let $\tilde{\mathbf{y}} = \mathbf{A}\tilde{\mathbf{x}}$. We easily obtain

$$\begin{aligned} |y_i - \tilde{y}_i| \exp(-\gamma_1 t - \gamma_2 z_0) &\leq (\lambda_i / \gamma_1) ||\mathbf{x} - \tilde{\mathbf{x}}||, \quad i = 1, \dots, n, \\ |y_{n+1} - \tilde{y}_{n+1}| \exp(-\gamma_1 t - \gamma_2 z_0) &\leq \lambda_{n+1} / (\gamma_1 \gamma_2) ||\mathbf{x} - \tilde{\mathbf{x}}||, \\ |y_{n+2} - \tilde{y}_{n+2}| \exp(-\gamma_1 t - \gamma_2 z_0) &\leq (\lambda_{n+2} / \gamma_1) ||\mathbf{x} - \tilde{\mathbf{x}}||, \\ |y_{n+3} - \tilde{y}_{n+3}| \exp(-\gamma_1 t - \gamma_2 z_0) &\leq (\lambda_{n+3} / \gamma_2) ||\mathbf{x} - \tilde{\mathbf{x}}||, \\ |y_{n+4} - \tilde{y}_{n+4}| \exp(-\gamma_1 t - \gamma_2 z_0) &\leq (\lambda_{n+4,1} / \gamma_1) ||\mathbf{x} - \tilde{\mathbf{x}}|| \\ &\quad + (\lambda_{n+4,2} / \gamma_1) ||\mathbf{x} - \tilde{\mathbf{x}}|| + \lambda_{n+4,3} T ||\mathbf{x} - \tilde{\mathbf{x}}||. \end{aligned}$$

Hence,

$$||\mathbf{y} - \tilde{\mathbf{y}}|| \leq \Lambda ||\mathbf{x} - \tilde{\mathbf{x}}||,$$

where

$$\Lambda = \varepsilon + \lambda_{n+4,3} T,$$

and

$$\varepsilon = \frac{1}{\gamma_1} \sum_{i=1}^n \lambda_i + \frac{\lambda_{n+1}}{\gamma_1 \gamma_2} + \frac{\lambda_{n+2}}{\gamma_1} + \frac{\lambda_{n+3}}{\gamma_2} + \frac{\lambda_{n+4,1}}{\gamma_1} + \frac{\lambda_{n+4,2}}{\gamma_1}.$$

The positive constants γ_1 and γ_2 were not specified earlier. Therefore, they can be chosen very large so that ε becomes very small. In addition, if $T < (1 - \varepsilon) / \lambda_{n+4,3}$, then $\Lambda < 1$, proving the theorem. \square

Remark 5.1 Let us note that the theorem provides the functions $x_i(z_0, t)$, $i = 1, \dots, n$, and $U(z_0, t)$. On the other hand the original problem required the the functions $X_i(z, t)$ and $u(z, t)$. This question is solved by Property 1, Sect. 4, where it is shown that the function $z = c(z_0, t)$ can be inverted and gives $z_0 = c^{-1}(z, t)$.

6 Substrates

In this section we generalize the free boundary problem stated in Sect. 2 by considering the equations for substrates which diffuse into the biofilm. Therefore, we assume

$$r_{M,i} = r_{M,i}(z, t, \mathbf{X}, \mathbf{S}), \quad \mathbf{S} = (S_1, \dots, S_m), \quad i = 1, \dots, n. \quad (6.1)$$

The diffusion of substrates from bulk liquid into the biofilm is governed by the following parabolic equations

$$\frac{\partial S_j}{\partial t} - D_j \frac{\partial^2 S_j}{\partial z^2} = r_{S,j}(z, t, \mathbf{X}, \mathbf{S}), \quad 0 < z < L(t), \quad j = 1, \dots, m, \quad t > 0, \quad (6.2)$$

where D_j denotes the diffusion coefficient of substrate j and $r_{S,j}(z, t, \mathbf{X}, \mathbf{S})$ is the production rate of substrate j . This equation is usually considered at pseudo-steady state conditions as the time-scale of substrate mass transport and reaction is orders of magnitude shorter than that of biomass spreading [5]

$$-D_j \frac{\partial^2 S_j}{\partial z^2} = r_{S,j}(z, \mathbf{X}, \mathbf{S}), \quad 0 < z < L(t), \quad j = 1, \dots, m, \quad t \geq 0. \quad (6.3)$$

The following boundary conditions will be associated to the equation above

$$\frac{\partial S_j}{\partial z}(0, t) = 0, \quad S_j(L(t), t) = S_j^*(t), \quad j = 1, \dots, m, \quad t \geq 0. \quad (6.4)$$

The first boundary condition in (6.4) prescribes zero substrate flux at the support $z = 0$. The second condition states that the substrate values on the moving boundary $z = L(t)$ are the same as the bulk liquid. The second condition strongly depends on the biological problem and Robin conditions could be assigned as well. However, this would not introduce further difficulties in the mathematical analysis.

Integrating (6.3) with boundary conditions (6.4) yields

$$S_j(z, t) = D_j^{-1} \int_z^L d\eta \int_0^\eta r_{S,j}(\zeta, \mathbf{X}(\zeta, t), \mathbf{S}(\zeta, t)) d\zeta + S_j^*(t), \quad 0 < z < L(t). \quad (6.5)$$

Integral Eq. (6.5) is equivalent to problem (6.3)–(6.4), since the boundary conditions are included in (6.5). For $z = c(z_0, t)$, Eq. (6.5) is rewritten as

$$S_j(c(z_0, t), t) = D_j^{-1} \int_{c(z_0, t)}^{c(w, t)} d\eta \int_0^\eta r_{S,j}(\zeta, \mathbf{X}(\zeta, t), \mathbf{S}(\zeta, t)) d\zeta + S_j^*(t), \quad 0 < z_0 < L_0, \quad j = 1, \dots, m, \quad (6.6)$$

where definition (3.15) was used. Now, consider the change of variables

$$\eta = c(\eta_0, t), \quad \zeta = c(\zeta_0, t), \quad 0 < \eta_0, \zeta_0 < L_0, \quad (6.7)$$

in (6.6) and obtain

$$s_j(z_0, t) = D_j^{-1} \int_{z_0}^w \frac{\partial c}{\partial \eta_0}(\eta_0, t) d\eta_0 \int_0^{\eta_0} r_{S,j}(c(\zeta_0, t), \mathbf{x}(\zeta_0, t), \mathbf{s}(\zeta_0, t)) \frac{\partial c}{\partial \zeta_0}(\zeta_0, t) d\zeta_0 + S_j^*(t), \quad 0 < z_0 < L_0, \quad j = 1, \dots, m, \quad (6.8)$$

where notation (3.6) was used and in addition

$$\mathbf{s}(z_0, t) = \mathbf{S}(c(z_0, t), t). \quad (6.9)$$

Note that integral Eq. (6.8) is similar to the integral equations considered in Sect. 5. Therefore, under assumption (6.1), Eq. (6.8) can be associated to system (5.2)–(5.6) and a general existence and uniqueness theorem can be proved as in Sect. 5 with small modifications.

7 Conclusion

A free boundary value problem for the detachment process in multispecies biofilm was discussed. The biological situation is related to mature biofilms where the detachment is the only relevant flux between biofilm and bulk liquid. Interesting properties for the solutions were derived. Uniqueness and existence theorem was proved. Of course other relevant questions should be investigated, e. g. the generalization to problems regarding more complex biological cases and stability problems, [16, 17].

However, the most fascinating objective before us is the qualitative analysis of the free boundary value problems for 2D and 3D biofilm growth models. We have some hope that the methodology used in this work could help.

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